Abstract

A method of comparing two conformers in which an overlay score is obtained, comprises providing a set of field points representing field extrema of a first molecule, wherein each field point has a position and a field size value; determining at the position of each of the field points of the first molecule the field of a second molecule to obtain a set of field sample values; and combining the field sample values with the field size values to obtain a score indicative of the field similarity of the first molecule to the second molecule. The method overcomes a limitation of conventional pseudo-Coulombic scoring in which a low score is achieved when extrema of large extent overlap but have their minimum points widely separated. The method can be applied to molecular mechanics modeling using atom centered charges (ACCs) and extended electron distributions (XEDs) as well as to quantum mechanics models.